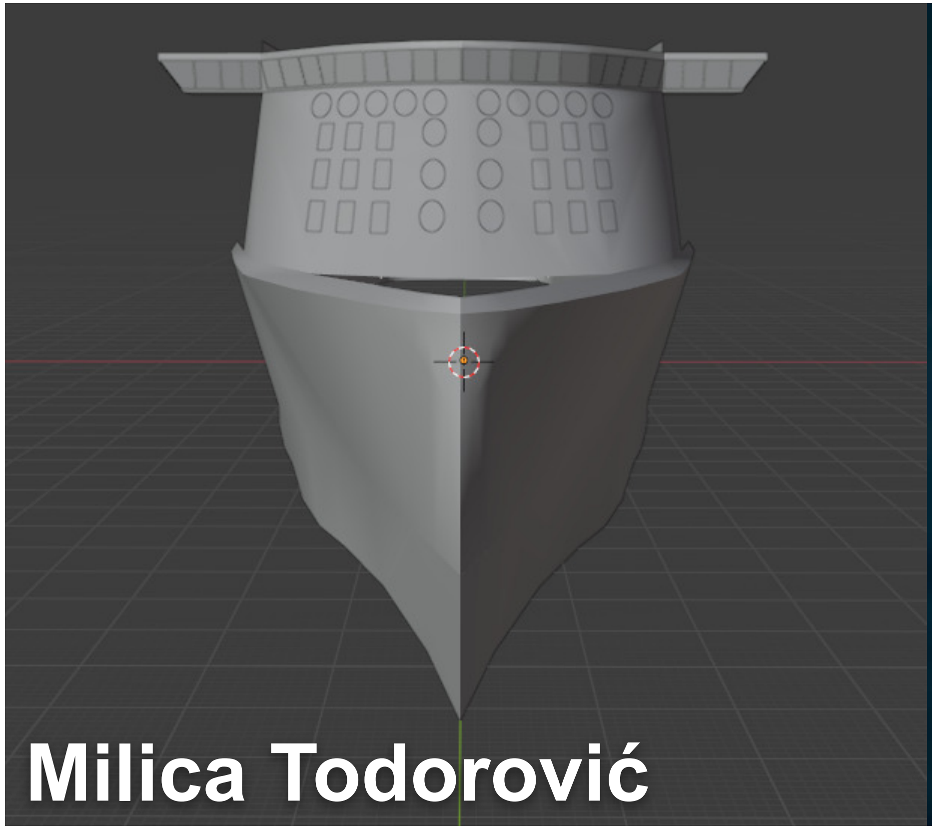
AI opportunities in digital ship hull design with LUMI supercomputing



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Materials Informatics Laboratory

- research objectives: combine artificial intelligence with computational and experimental materials data to accelerate discovery
- application areas: energy (solar cells, batteries), health (atmospheric chemistry, sensor development) and manufacturing technology (process optimization, Design of Experiments)
- part of FCAI (Highlight E: AI-driven design of materials) and Sustainable Materials and Manufacturing centre (SUSMAT)
- AI in the industry and classroom: “Machine Learning for Materials Science”

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Artificial intelligence to accelerate discovery

materials science data

100100101
010010010
101110111
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training →

AI model

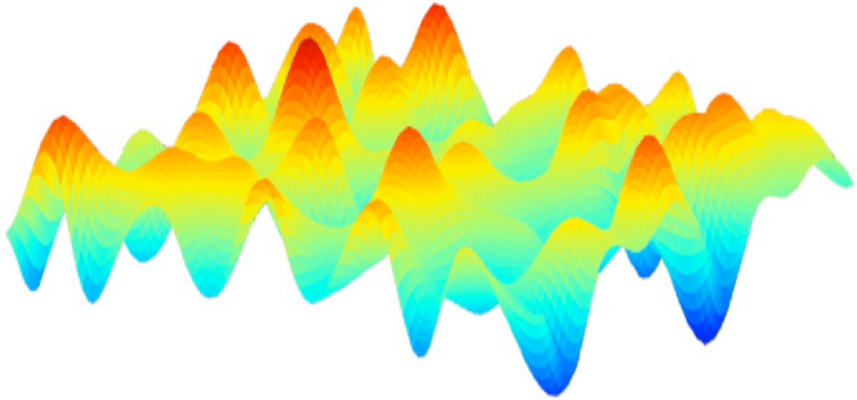
predicting →

new insight

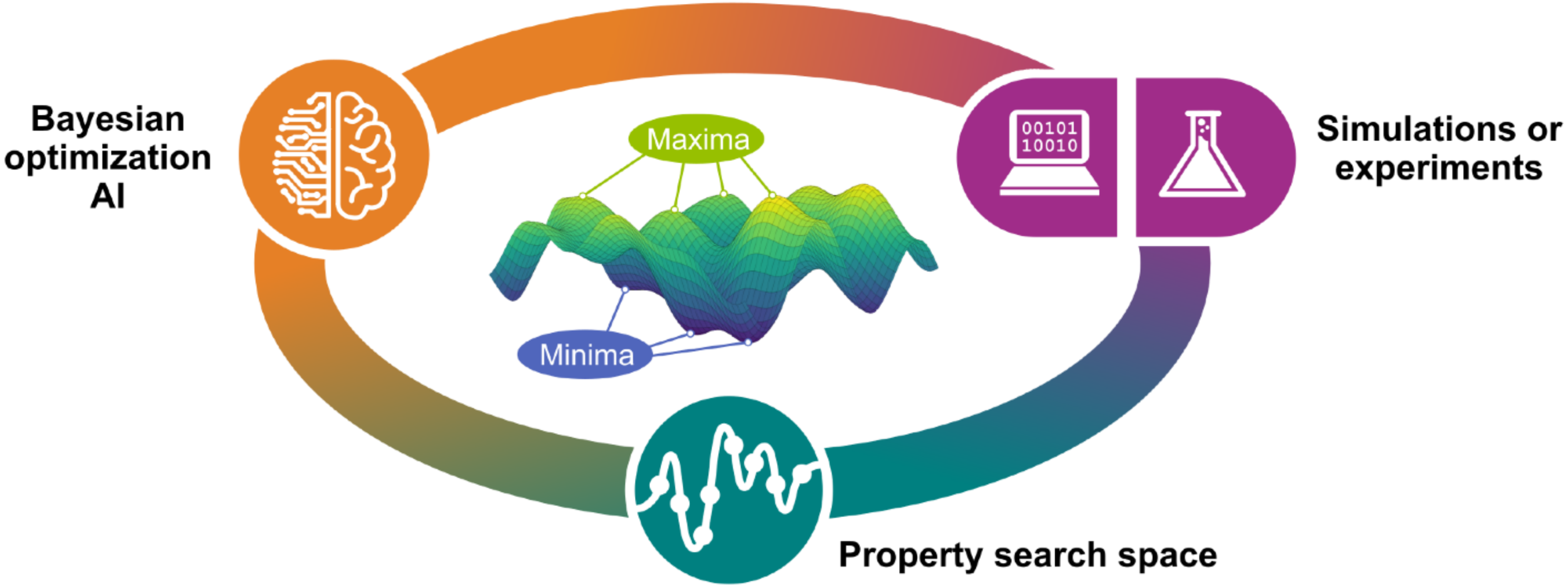
AI applications in materials science:

- data analytics
- pre-screening & materials design
- device tuning and optimization
- guiding experimental work

structure-property landscape



Bayesian Optimisation Structure Search (BOSS)



Active learning engine for materials optimisation

www.utu.fi/boss

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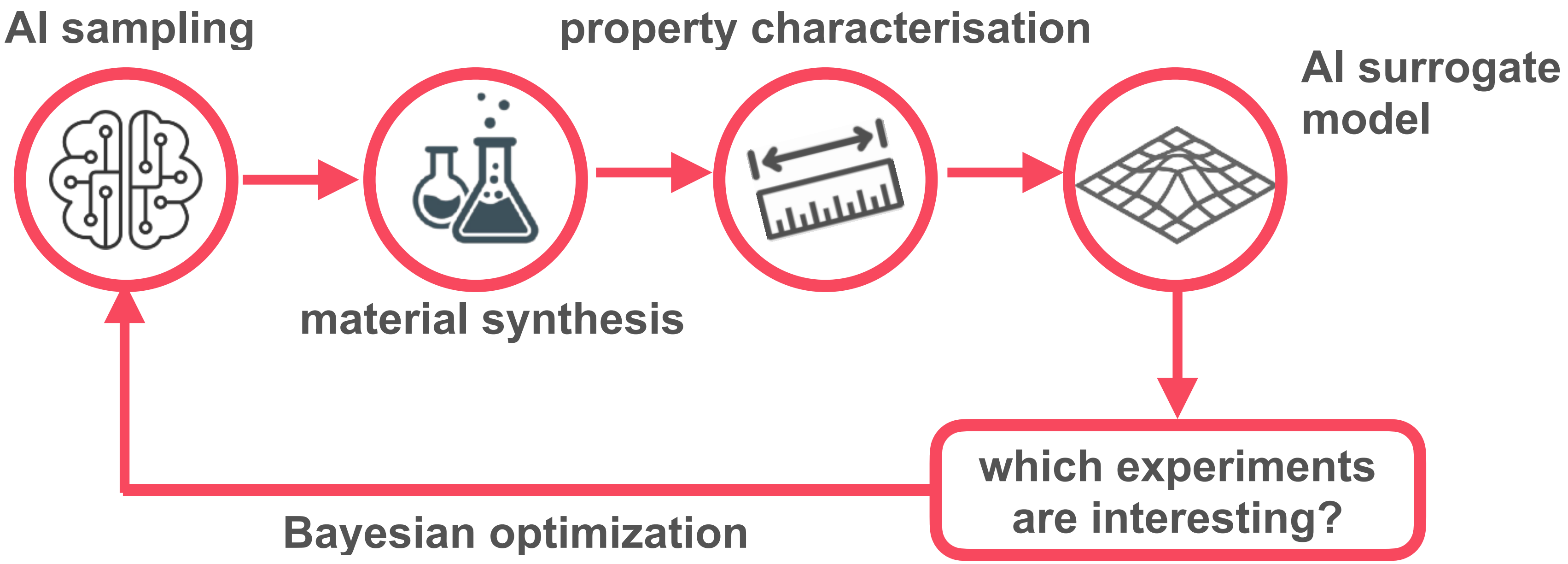
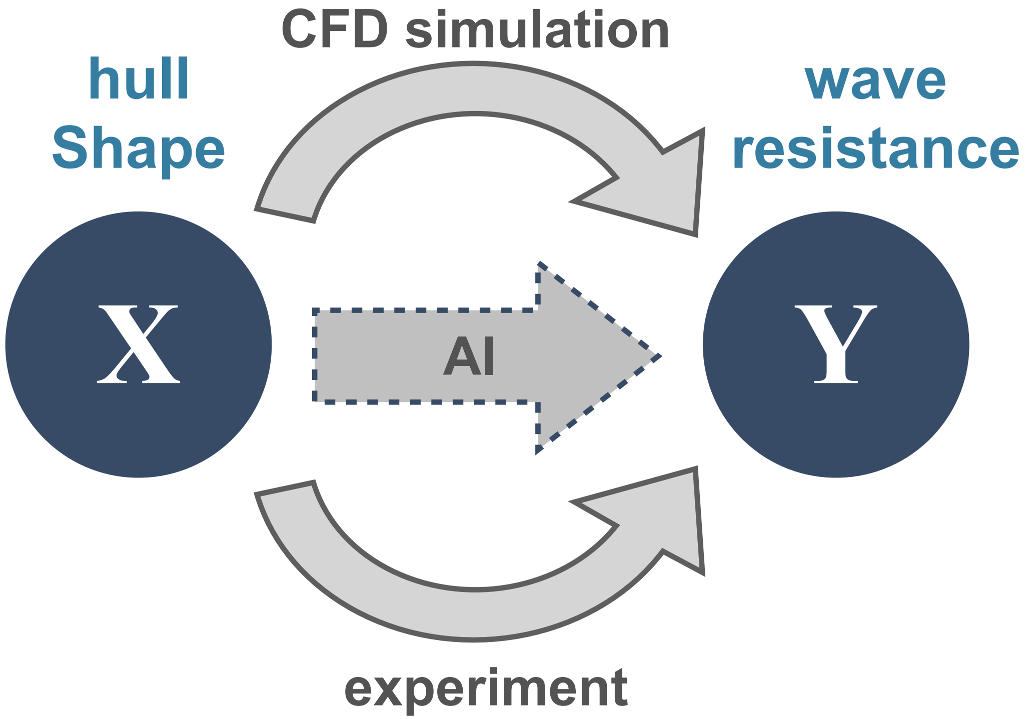
BOSS for guiding experiments

Bayesian Optimization **guides experimental data collection** to develop **predictive models** (possibly high-dimensional) and **optimize target properties,** while conducting **as few experiments as possible.**



AI-guided ship hull optimisation

- ship hull optimisation is complex: too many variables and design choices
- computational fluid dynamics (CFD) is costly: big data is not feasible
- LUMI solutions: automated workflows
- AI objectives: to identify hull shapes that minimise water resistance



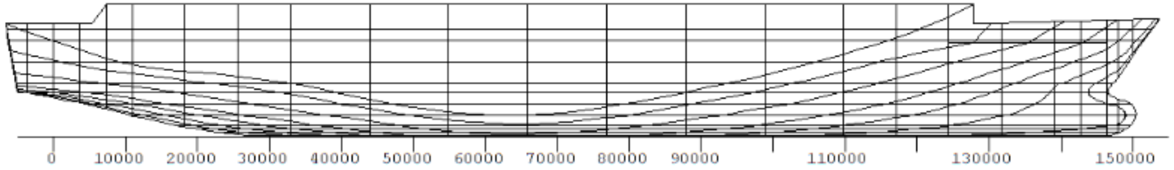
AI challenges

- **Design space:** how to define the search space of hull shape deformations?
- **Hull representation**: how to describe the hull shape to the AI algorithm?
- **Computational implementation**: how to automate sampling of hull shapes?
- **AI algorithms**: how to guide the search to optimal solutions with limited budget?

Hull shape representation

CFD inputs and data types:

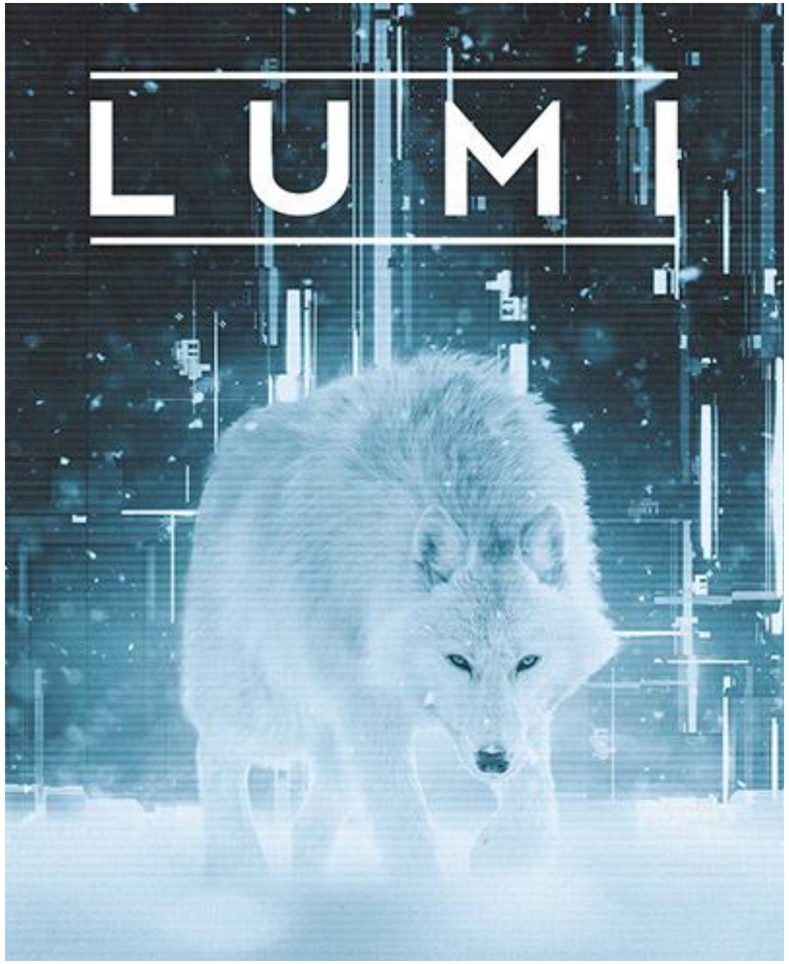
- hull data: vector or matrix
  - up to 6000 input data
  - 100 frame, 200 waterline, 200 vertical
  - possibility to downsize data
- speed: scalar numerical
- draught: scalar numerical



Representation

Computational implementation

- generate data set based on CFD simulations of different ship hulls sampled
- openFOAM implementation on LUMI + AI tools
- each data entry: [x, y] pair, where:
    - [x] - ship hull and simulation conditions
    - [y] - simulation output: wave resistance
- AI model to map [x] ➡ [y], and conduct a search



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Deploying AI and big data in the industry

Metso

Big data analytics of recycling

SmartCycling Academy Project
(Research Council of Finland 2022-26)

UTU donation funds

MEYER TURKU
SHIPYARD 1737

Optimizing ship hull design for energy efficiency

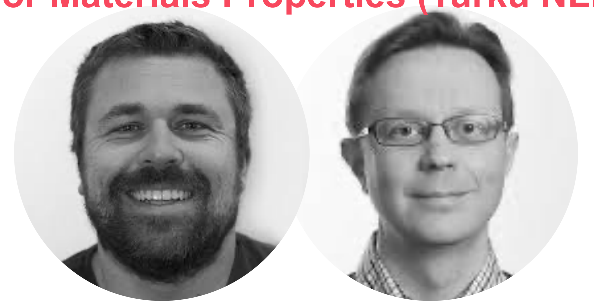
Research Council of Finland

CSC

ICT Solutions for Brilliant Minds

BUSINESS FINLAND

Natural Language Processing for Materials Properties (Turku NLP)



DeeperMaterials Academy Project
(Research Council of Finland 2021-24)

BOSS web application

storaenso

(Business Finland pending)

Optimising optical coatings

SENOP

SmartFab Co-Innovation
(Business Finland 2024-26)

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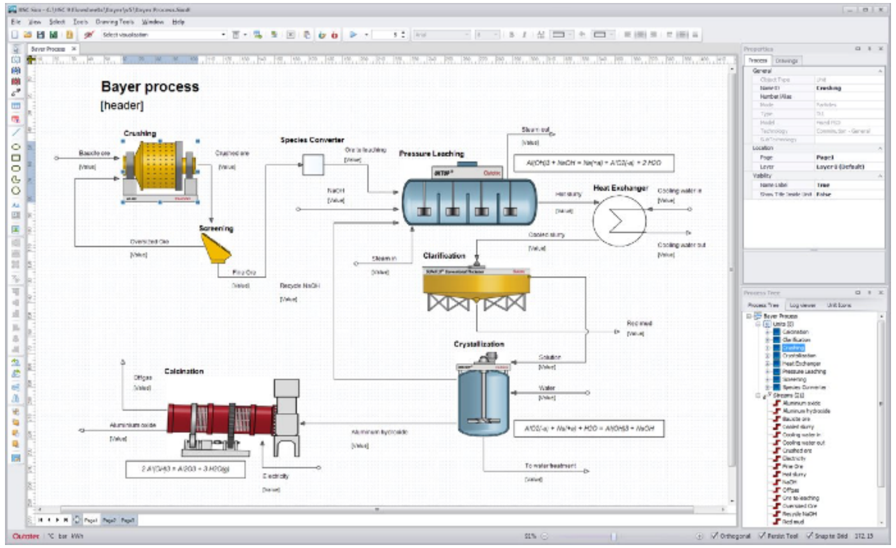
Materials recovery from battery recycling

Metso



HSC-Sim package:
Simulated materials processing

traditional

Use Graphical User Interface
Visualise process
Optimise process manually

innovative

Use API + Python libraries
Deploy parallel simulations
AI-driven process optimisation

Optimising the circular economy of batteries with artificial intelligence aided designs (SmartCycling)
Research Council of Finland (2022-2026)

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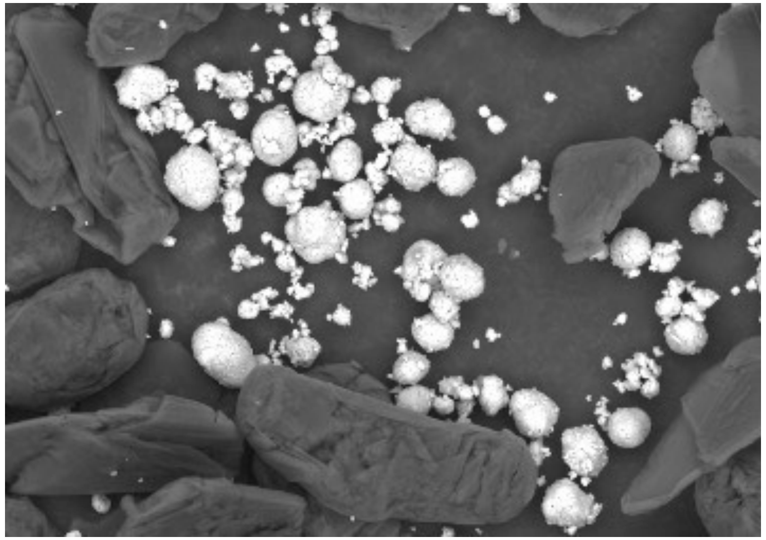
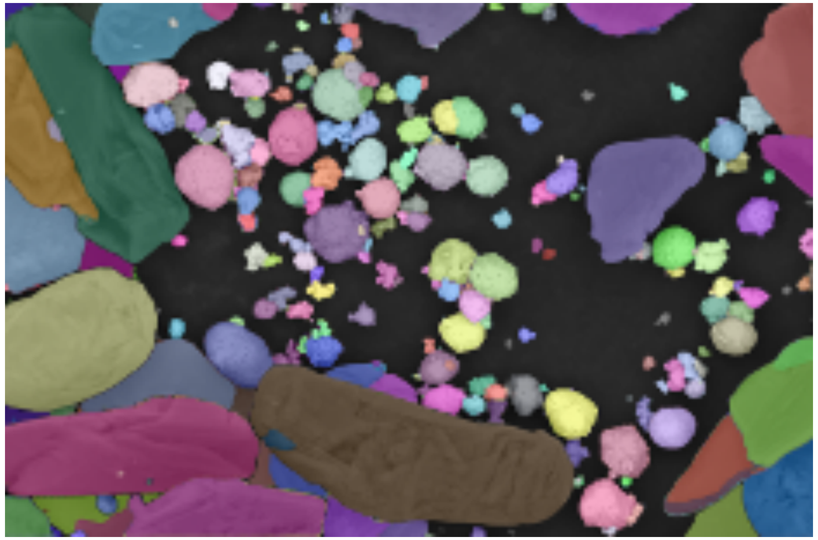
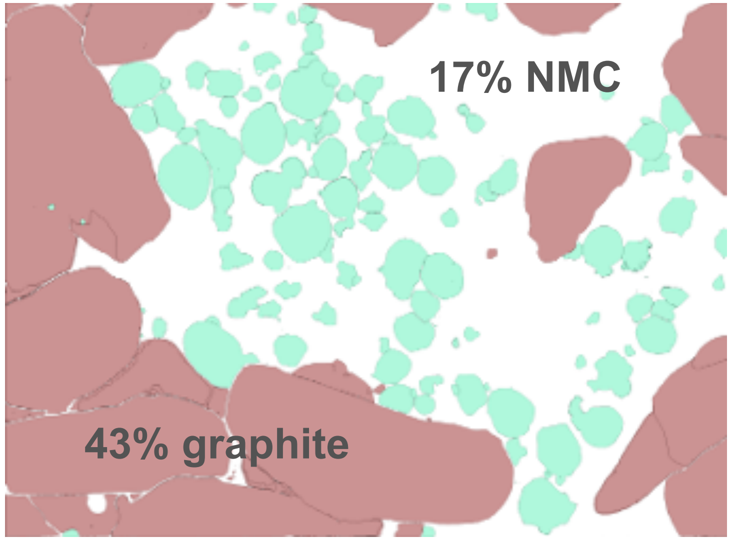
Materials recovery with image processing

Can we learn the materials composition of crushed battery waste from microscopy images?







1. Microscopy image
Battery cathode (NMC, white)
Battery anode (graphite, dark)

2. Image segmentation:
Identifying individual particles of different materials

3. Material identification
Assigning material type to individual particles

Optimising the circular economy of batteries with artificial intelligence aided designs (SmartCycling)
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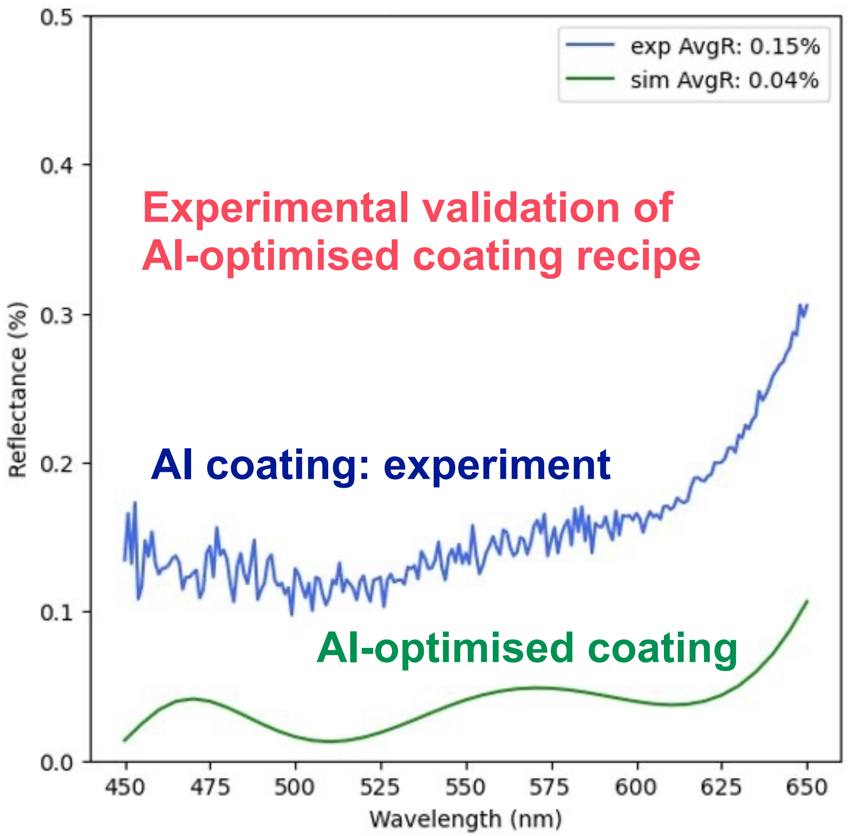
Big data for anti-reflective coatings

- optical coating performance depends on materials, layer thickness, ordering, etc.
- simulations avoid trial-and-error experiments
- traditional tools: Windows and GUI-based, difficult for extensive optimisation
- switch to new open-source tools: millions of data produced on the CSC
- ultra-low reflectance found and manufactured



SmartFab Co-Innovation Grant (Business Finland 2024-26)

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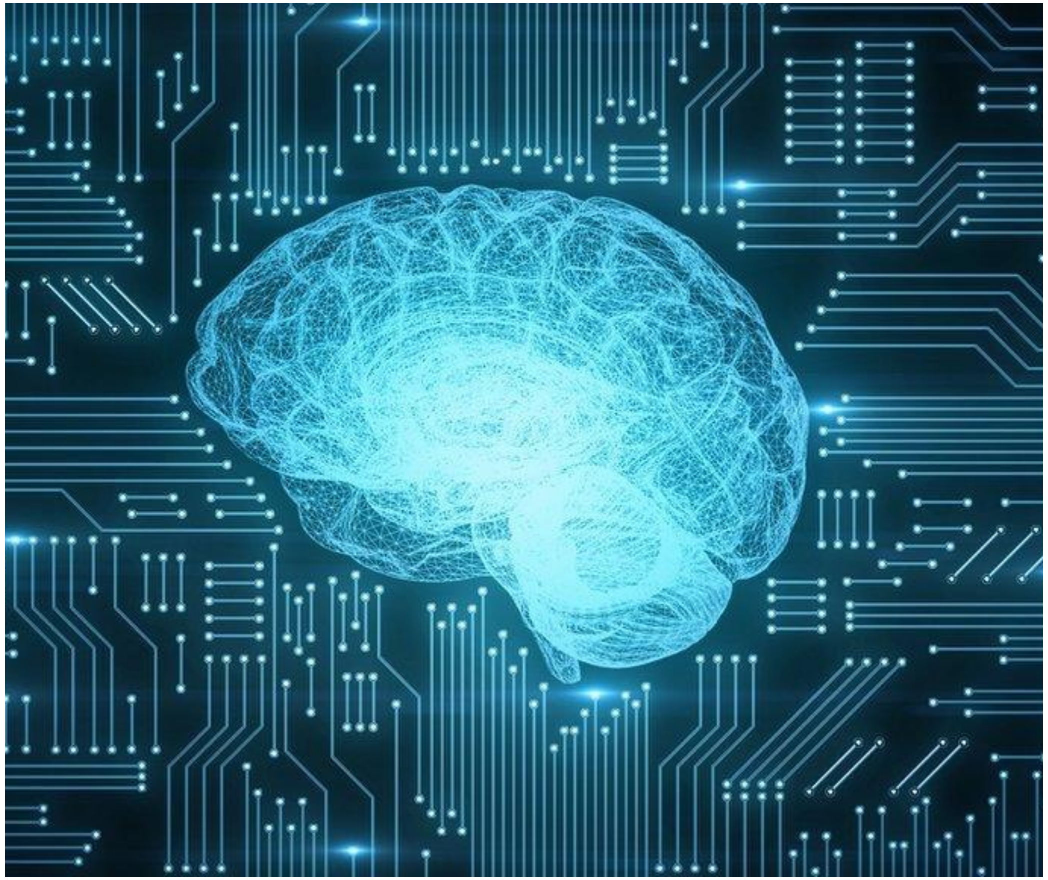
AI opportunities waiting to be unlocked!



- Finnish industry is slow to benefit from AI
- big opportunities in R&D: product development
- CSC HPC computing and new codes are central to AI-driven workflows
- new tools and education are important to democratise AI and lower barriers for use
- more companies should follow Meyer: consult with AI experts & CSC about custom solutions

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